

Carbon tetrachloride

56-23-5 | DTXSID8020250

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 63.5 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.49e-01

Confidence level: 5.43e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Carbon tetrachloride</div> <div>Measured: 115</div> <div>Predicted: 63.5</div>	<div>Image not found</div> <div>Dibromodifluoromethane</div> <div>Measured: 39.0</div> <div>Predicted: 781</div>	<div>Image not found</div> <div>1-Chloro-2-propanol</div> <div>Measured: 18.5</div> <div>Predicted: 5.24</div>
<div>Image not found</div> <div>Dimethyl sulfoxide</div> <div>Measured: 2.10e-01</div> <div>Predicted: 3.98e-01</div>	<div>Image not found</div> <div>Trimethylamine</div> <div>Measured: 803</div> <div>Predicted: 862</div>	